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## Controlling the Biological Effects of Spermine Using a Synthetic Receptor

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**Supporting Information for:**

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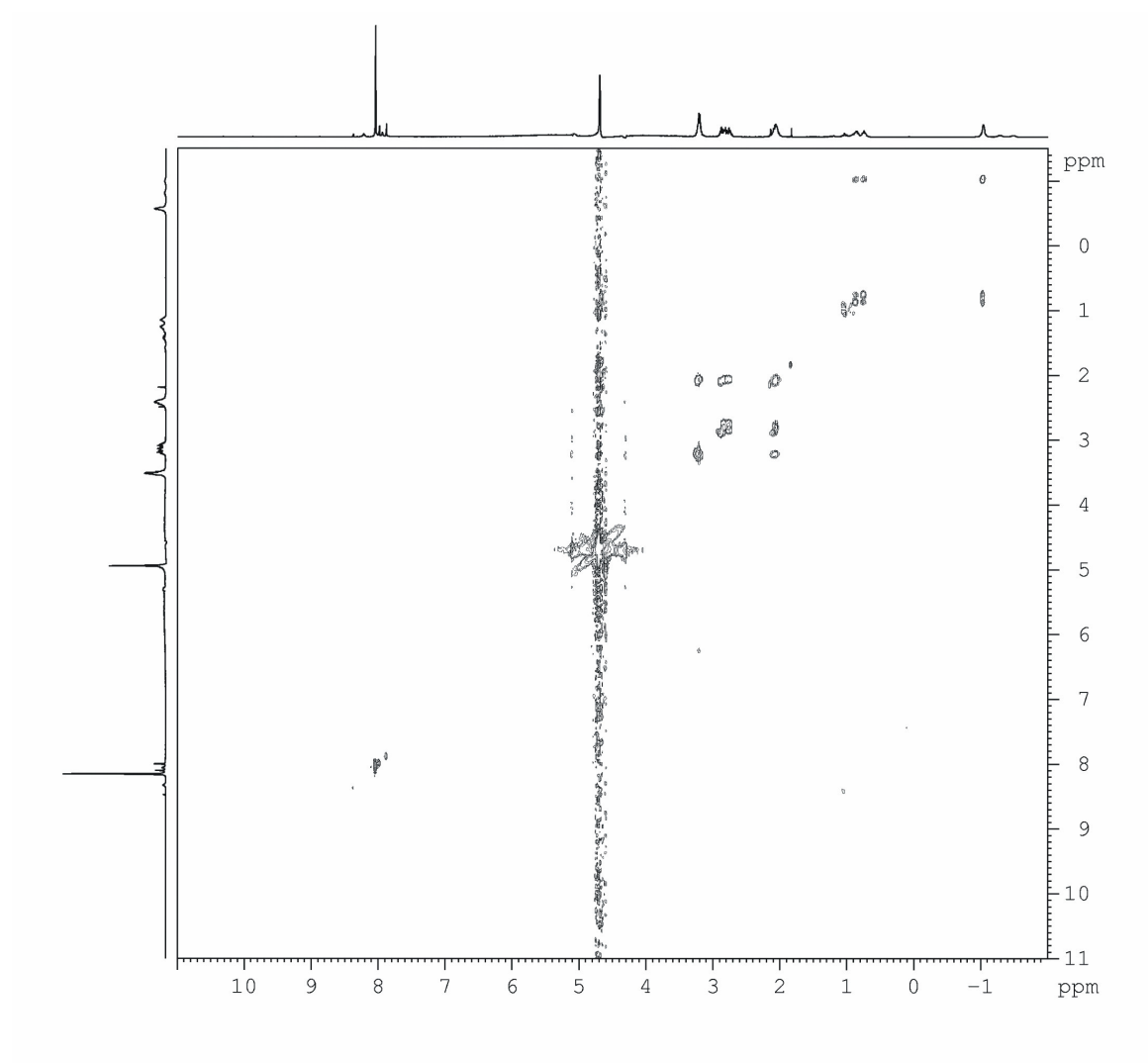
*Laurent Vial, R. Frederick Ludlow, Julien Leclaire, Ruth Pérez-Fernández, Sijbren  
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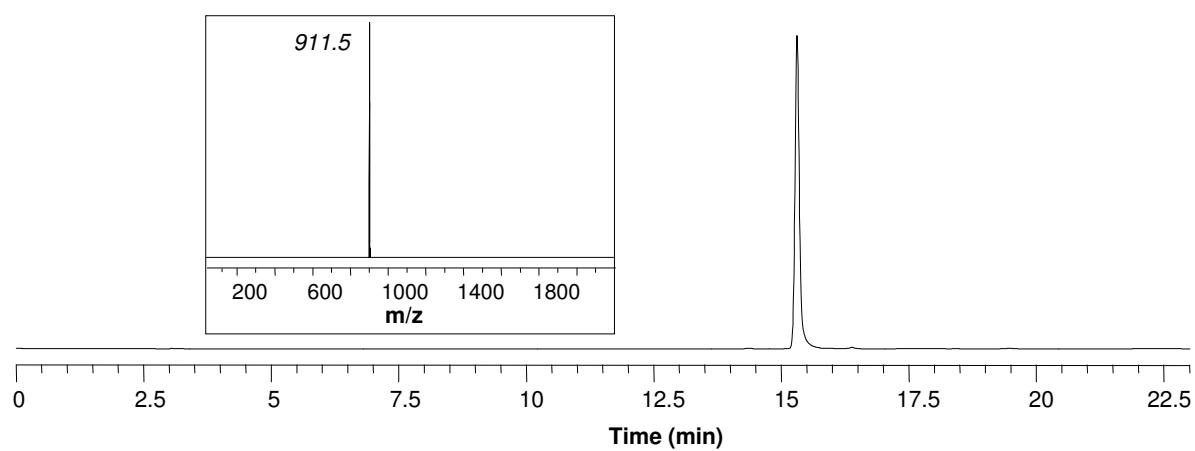
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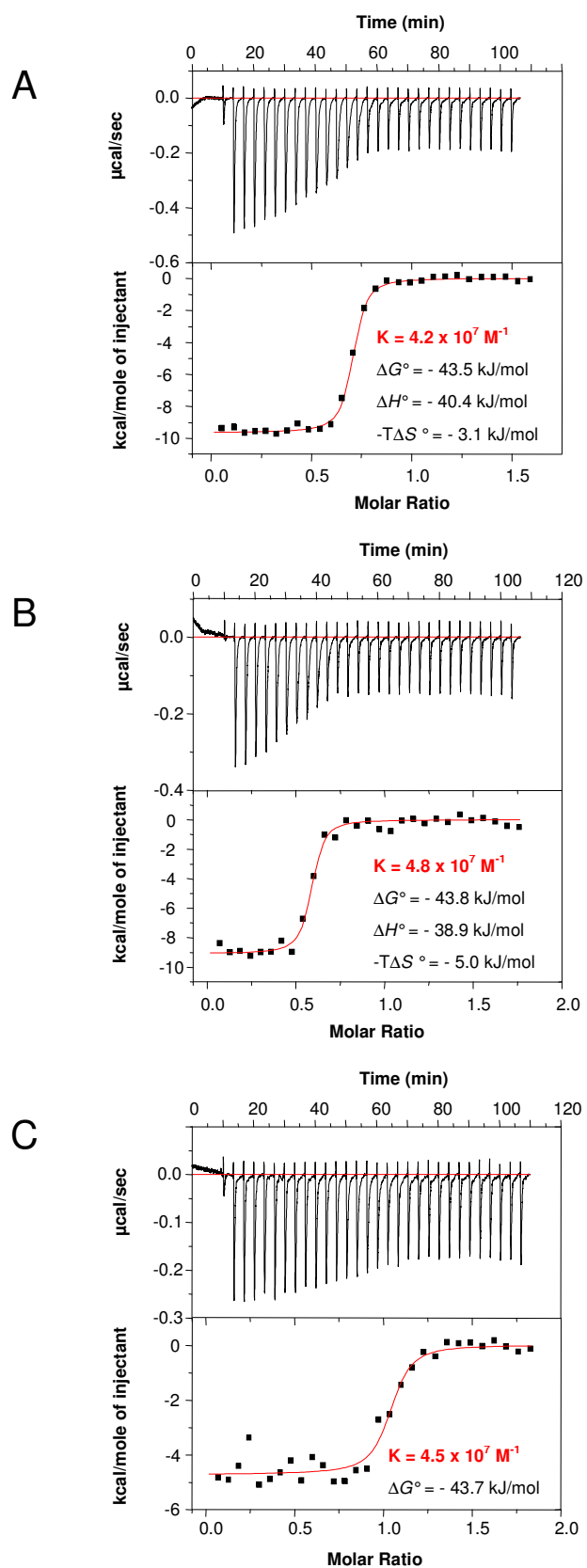
COSY spectrum of the complex between spermine and <b>6</b> .	S2
LC-MS analysis of <b>6</b> .	S2
ITC studies of binding of spermine to <b>6</b> .	S3
Computer simulation results.	S4



**Figure S1.** COSY spectrum of the complex between spermine and **6**. Solvent: 89 mM phosphate buffer (pH 7.4, 11% D<sub>2</sub>O)



**Figure S2.** HPLC and MS (inset) analysis of **6**.



**Figure S3.** ITC data. Concentrations of **1** and **6** are 0.1068 mM and 0.0156 mM (A), 0.0739 mM and 0.0098 mM (B), 0.0528 mM and 0.0070 mM (C) respectively.

**Table S1.** Energies of the free receptors and complexes as determined by molecular dynamics simulations.

<i>Species</i>	<i>Relative configurations of the disulfide bonds</i>	<i>MD Energies Average Total Energy (kJmol<sup>-1</sup>)</i>	<i>Relative MD Energies<sup>(a)</sup> (kJmol<sup>-1</sup>)</i>
Receptor	(P,P,P,P)	-1785.89	5.83
	(P,P,P,M)	-1786.73	4.99
	(P,P,M,M)	-1784.50	7.22
	(P,M,P,M)	-1791.72	0
Complex	(P,P,P,P)	-2735.61	0
	(P,P,P,M)	-2718.94	16.67
	(P,P,M,M)	-2715.36	20.25
	(P,M,P,M)	-2693.90	41.71

(a) MD energy relative to the most stable stereoisomer.